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INITIAL RESEARCH ON CHEMICAL CONSTITUENTS OF *CURCUMA SINGULARIS* RHIZOMES

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ABSTRACT

From the rhizomes of *Curcuma singularis* Gagnep (Zingiberaceae family), six compounds, including three terpenoids, *p*-menthane-1,2,4-triol (**1**), amoxantin A (**2**), rugosic acid B (**3**); two diols, 2,3-butanediol (**4**) [*2R,3R*-butanediol (**4a**) and *2S,3S*-butanediol (**4b**)], and *meso*-2,3-butanediol (**5**), along with 3-hydroxy-4-methoxy benzoic acid (**6**) were isolated. All of six compounds were obtained for the first time from the *Curcuma* genus. The structures of those compounds were determined by 1D and 2D-NMR spectroscopic data.

Keywords: Curcuma singularis Gagnep., Zingiberaceae, rhizomes, terpenoid, labdadien, butanediol, benzoic acid.

1. INTRODUCTION

Curcuma is a large genus belonging to Zingiberaceae family, comprise of 147 species over the world [1] and 15 species in Vietnam [2]. Several *Curcuma* species were used in traditional medicine for the treatment of gastrointestinal disorders, abdominal pain, jaundice, and hepatitis [3]. *Curcuma singularis* Gagnep., local name "cây khỏe" were used by ethnic people in Tay Nguyen provinces as medicinal remedy for increasing vitality, boosting health, treating rheumatism and fortifying kidney.

Around the world, so far there have been many publications on the chemical compositions and biological activity of the *Curcuma* species such as *Curcuma longa* L. [4, 5], *C. wenyujin* [6], and *C. comosa* [7]. Compounds mainly found in this genus were tecpenoids and diaryl phenyls [4 - 7]. However, to the best of our knowledge, there are not any studies announced on the chemical compositions and biological activity of *C. singularis*. In this paper, we present some our initial findings on the chemical compositions of the rhizomes of *Curcuma singularis* Gagnep.

2. MATERIALS AND METHODS

2.1. Plant material

The rhizomes of *C. singularis* were collected in Kon Pne commune, K'bang distrist, Gialai province, Vietnam in April 2015. The plant was identified by botanist Dr. Nguyen Quoc Binh, Institute of Ecology and Biological Resources (VAST), Vietnam. A voucher specimen (C-557) is deposited in the Herbarium of the Institute of Natural Products Chemistry (VAST), Hanoi, Vietnam.

2.2. General experimental procedures

^{1}H-NMR (500 MHz) and ^{13}C-NMR (125 MHz) were measured on a Bruker Avance 500 MHz spectrometer, Institute of Chemistry. ESI-MS were obtained from an Agilent 1100 Series LC/MSD Trap SL, Institute of Chemistry. Chromatographic separation was carried out on silica gel (Si 60 F_{254}, 40-63 mesh, Merck) and RP-C_{18} column. All solvents were redistilled before use. Pre-coated TLC plates (Si 60 F_{254}) were used for analytical purposes.

2.3. Extraction and isolation

Dried powdered rhizomes of *C. singularis* (3.2 kg) were extracted with ethanol 80^{o} (3 × 7L) at room temperature and concentrated under reduced pressure to yield a black crude ethanol extract (300 g). The crude ethanol extract was suspended in hot ethanol-water (1:1, v/v) and successively partitioned with chloroform, ethyl acetate and water. The resulting fractions were concentrated under reduced pressure to give the corresponding solvent-soluble fractions chloroform (198 g, CS-C), ethyl acetate (6.0 g, CS-E) and water (96 g, CS-W).

The chloroform fraction (CS-C, 198 g) was chromatographed on a silica gel column, using solvent gradient of *n*-hexan : ethyl acetate (6:1, v/v) to afford 8 fractions (C1-C8). The fraction C1 (15 g) was chromatographed on a silica gel column, eluting with *n*-hexane : ethyl acetate (100:1, v/v) to afford 4 subfractions (C1A-C1D). Precipitate from C1C subfraction (3.5 g) was filtered and washed to yield compound **2** (100 mg). The fraction C5 (1.59 g) was chromatographed on a silica gel column, eluting with dichloromethane : acetone (20/1, v/v) to afford 7 subfractions (C5A-C5G). The subfraction C5E (243 mg) was eluted with isocratic solvent system of *n*-hexane : acetone (5:1, v/v) on a silica gel column to yield compound **1** (4 mg).

The ethyl acetate fraction (CS-E, 6.0 g) was subjected for chromatography column (CC) on a flash silica gel column (400-630 mesh), eluting with chloroform-acetone (10:1, v/v) to afford 11 fractions (E1-E11). The fraction E2 (110 mg) was chromatographed on a silica gel column, eluting with chloroform : ethyl acetate (10:1, v/v) to afford 2 subfractions (E2A-E2B). Precipitate from E2A (80 mg) was filtered and washed with chloroform to yield compound **6** (10.0 mg). The fraction E10 (220 mg) was chromatographed on a silica gel column, eluting with ethyl acetate : methanol (5:1, v/v) to afford 5 subfractions (E10A-E10E). The subfraction E10B (25 mg) was rechromatographed over a RP-18 column eluting with methanol : water (1:1, v/v) to yield compound **3** (6 mg).

The water fraction (CS-W, 96 g) was subjected to a Diaion CC, eluting with gradient solvent mixture of water-methanol (1:0→0:1) to produce 5 fractions (W1-W5). The fraction W1 (70 g) was purified on a silica gel CC using chloroform : methanol : water (6:1:0.1, v/v) to

afford 11 fractions (W1A-W1J). The subfraction W1A (1.6 g) was chromatographed on a silica gel column, eluting with chloroform : acetone (6:1, v/v) to afford 5 subfractions and yield compound **4** (100 mg) and compound **5** (80 mg).

***p*-menthane-1,2,4-triol** (**1**): White needle crystals ($C_{10}H_{20}O_3$). ^{1}H-NMR (500 MHz, MeOD), δ_H (ppm): 0.93 (3H, d, J = 7.0 Hz, H-9), 0.94 (3H, d, J = 7.0 Hz, H-8), 1.26 (3H, s, 1-CH_3), 1.44 (2H, m, H-6), 1.60 (1H, dd, J = 13.0, 6.5 Hz, H-7), 1.63 (1H, dt, J = 14.0, 3.0 Hz, H_a-3), 1.85 (1H, dd, J = 13.5, 4.0 Hz, H_a-5), 1.93 (1H, dd, J = 13.5, 3.5 Hz, H_b-5), 1.96 (1H, dt, J = 14.0, 3.5 Hz, H_b-3), 3.53 (1H, brs, H-2). ^{13}C-NMR (125 MHz, MeOD), δ_C (ppm): 17.1 (q, C-9), 17.2 (q, C-8), 27.1 (q, 1-CH_3), 30.3 (t, C-6), 30.4 (t, C-5), 34.9 (t, C-3), 39.0 (d, C-7), 72.1 (s, C-1), 75.7 (s, C-4), 75.7 (d, C-2).

Amoxantin A (**2**): Yellowish needle crystals ($C_{18}H_{28}O$). ^{1}H-NMR (500 MHz, $CDCl_3$), δ_H (ppm): 0.85 (3H, s, H-19), 0.89 (6H, s, H-18, H-20), 1.02 (1H, ddd, J = 3.0, 13.0, 13.0 Hz, H_a-1), 1.10 (1H, dd, J = 2.5, 12.5 Hz, H-5), 1.19 (1H, ddd, J = 4.5, 13.5, 14.0 Hz, H_a-3), 1.37 (1H, m, H_b-1), 1.39 (1H, m, H_a-6), 1.41 (1H, m, H_a-2), 1.44 (1H, m, H_b-3), 1.54 (1H, m, H_b-2), 1.72 (1H, m, H_b-6), 2.09 (1H, ddd, J = 5.0, 12.5, 13.5 Hz, H_a-7), 2.27 (3H, s, H-14), 2.44 (1H, m, H_b-7), 2.47 (1H, m, H-9), 4.41 (1H, d, J = 1.0 Hz, H_a-17), 4.79 (1H, d, J = 1.0 Hz, H_b-17), 6.07 (1H, d, J = 16.0 Hz, H-12), 6.87 (1H, dd, J = 6.0, 16.0 Hz, H-11). ^{13}C-NMR (125 MHz, $CDCl_3$), δ_C (ppm): 15.1 (q, C-20), 19.0 (t, C-2), 21.9 (q, C-19), 23.3 (t, C-6), 27.2 (q, C-14), 33.5 (s, C-4), 33.6 (q, C-18), 36.6 (t, C-7), 39.3 (s, C-10), 40.9 (t, C-1), 42.1 (t, C-3), 54.5 (d, C-5), 60.8 (d, C-9), 108.6 (t, C-17), 133.6 (d, C-12), 146.6 (d, C-11), 148.6 (s, C-8), 198.1 (s, C-13).

Rugosic acid B (**3**): Colorless crystals ($C_{15}H_{22}O_5$). ^{1}H-NMR (500 MHz, MeOD), δ_H (ppm): 0.94 (3H, d, J = 7.0 Hz, H-13), 1.02 (3H, d, J = 6.5 Hz, H-12), 1.15 (3H, s, 7-CH_3), 1.68 (1H, m, H_a-8), 1.71 (1H, m, H_a-9), 1.78 (1H, m, H_b-8), 1.92 (1H, d, J = 12.0 Hz, H_a-6), 2.02 (1H, d, J = 12.0 Hz, H_b-6), 2.06 (1H, m, H_b-9), 2.14 (1H, dd, J = 7.5, 3.0 Hz, H-10), 2.41 (1H, m, H-11), 4.02 (1H, d, J = 5.0 Hz, H-2), 6.63 (1H, d, J = 5.0 Hz, H-3). ^{13}C-NMR (125 MHz, MeOD), δ_C (ppm): 20.7 (q, C-13), 24.4 (t, C-9), 24.8 (q, 7-CH_3), 25.8 (q, C-12), 26.1 (d, C-11), 45.3 (t, C-8), 49.7 (s, C-7), 54.0 (d, C-10), 57.1 (t, C-6), 66.4 (d, C-2), 97.8 (s, C-1), 103.2 (s, C-5), 134.2 (d, C-3), 141.4 (s, C-4), 173.5 (s, CO).

2,3-butanediol (**4**): Yellowish oil ($C_4H_{10}O_2$). ^{1}H-NMR (500 MHz, MeOD), δ_H (ppm): 1.16 (6H, d, 6.0 Hz, H-1, H-4), 3.56 (2H, m, H-2, H-3). ^{13}C-NMR (125 MHz, MeOD), δ_C (ppm): 18.6 (q, C-1), 18.7 (q, C-4), 72.6 (d, C-2), 72.7 (d, C-3).

***meso*-2,3-butanediol** (**5**): Yellowish oil ($C_4H_{10}O_2$). ^{1}H-NMR (500 MHz, MeOD), δ_H (ppm): 1.14 (6H, d, 6.5 Hz, H-1, H-4), 3.53 (2H, m, H-2, H-3). ^{13}C-NMR (125 MHz, MeOD), δ_C (ppm): 18.7 (q, C-1, C-4), 72.7 (d, C-2, C-3).

3-Hydroxy-4-methoxybenzoic acid (**6**): White needle crystals ($C_8H_8O_4$). ^{1}H-NMR (500 MHz, MeOD), δ_H (ppm): 3.91 (3H, s, H-8), 6.86 (1H, d, J = 8.5 Hz, H-5), 7.57 (1H, d, J = 2.5 Hz, H-2), 7.58 (1H, d, J = 2.5, 8.5 Hz, H-6). ^{13}C-NMR (125 MHz, MeOD), δ_C (ppm): 56.4 (q, 4-OCH_3), 113.8 (d, C-5), 115.8 (d, C-2), 123.1 (s, C-1), 125.3 (d, C-6), 148.7 (s, C-3), 152.7 (s, C-4), 170.0 (s, CO).

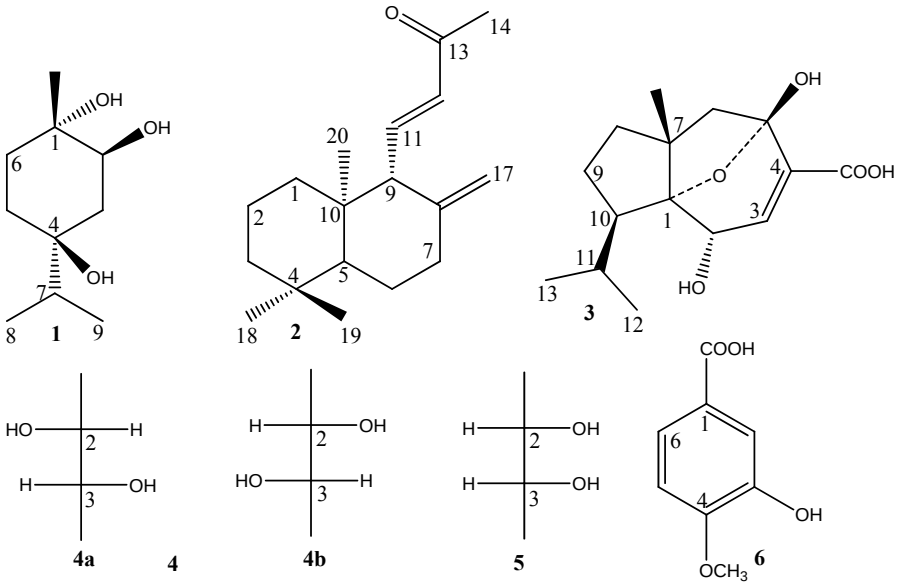

Figure 1. Compounds (**1-6**) from rhizomes of *Curcuma singularis* species.

3. RESULT AND DISCUSSION

Compound **1** was obtained as white needle crystals. The ^{1}H-NMR of **1** showed characteristic signals for a monoterpene, including two methyl protons of isopropyl group at [δ_H 0.93 (J = 7.0 Hz, H-9), δ_H 0.94 (J = 7.0 Hz, H-8)], one methyl group at δ_H 1.26 (1-CH_3), three methylene groups at [δ_H 1.44 (m, H-6), δ_H 1.85 (dd, J = 13.5, 4.0 Hz, H_a-5), δ_H 1.93 (dd, J = 13.5, 3.5 Hz, H_b-5), δ_H 1.63 (dt, J = 14.0, 3.0 Hz, H_a-3) and δ_H 1.96 (dt, J = 14.0, 3.5 Hz, H_b-3)], and two methine protons at [δ_H 1.60 (dd, J = 13.0, 6.5 Hz, H-7), δ_H 3.53 (brs, H-2)]. In agreement with those, ^{13}C-NMR/DEP of **1** showed 10 carbon signals, assignable to three methyl carbons at [δ_C 17.1 (q, C-9), δ_C 17.2 (q, C-8), δ_C 27.1 (q, 1-CH_3)], three methylene carbons at [δ_C 30.3 (t, C-6), δ_C 30.4 (t, C-5), δ_C 34.9 (t, C-3)], two methine carbons at [δ_C 39.0 (d, C-7), δ_C 75.7 (d, C-2)], and two quaternary carbons at [δ_C 72.1 (s, C-1), δ_C 75.7 (s, C-4)]. Analysis of HMBC spectra, methyl proton 1-CH_3 correlated to C-1, C-2 and C-6, which confirmed the position of methyl group at C-1. Similarly, isopropyl side chain at C-4 was confirmed by the HMBC correlations between H-8/H-9 and C-4/C-7. From 1D, 2D-NMR data, together with a comparison with spectral data in published literature, the chemical structure of **1** was elucidated as a polyoxygen-monoterpene with trivial name *p*-menthane-1,2,4-triol [8].

Compound **2** was isolated as yellowish needle crystals. The ^{1}H-NMR spectrum of **2** displayed patterns of diterpenoid, bicyclic skeleton of bisnorlabdane, with characteristic signals of three methyl groups at δ_H 0.85 (s, H-19), δ_H 0.89 (s, H-18, H-20), one exomethylene group at [δ_H 4.41 (d, J = 1.0 Hz, H_a-17), δ_H 4.79 (d, J = 1.0 Hz, H_b-17), one α, β-unsaturated ketone side chain at [δ_H 6.80 (dd, J = 10.0, 16.0 Hz, H-11), δ_H 6.07 (J = 16.0 Hz, H-12), δ_H 2.27 (s, H-14)]. ^{13}C-NMR/DEPT spectra of **2** contained 18 carbon signals, composed of four methyl groups at [δ_C 27.2 (q, C-14), δ_C 33.6 (q, C-18), δ_C 21.9 (q, C-19), δ_C 15.1 (q, C-20)], six methylene carbons at [δ_C 40.9 (t, C-1), δ_C 19.0 (t, C-2), δ_C 42.1 (t, C-3), δ_C 23.3 (t, C-6), δ_C 36.6 (t, C-7), δ_C 108.6 (t, C-17)], four methine carbons at [δ_C 54.5 (d, C-5), δ_C 60.8 (d, C-9), δ_C 146.6 (d, C-11), δ_C 133.6 (d, C-12)], three quaternary carbons at [δ_C 33.5 (s, C-4), δ_C 148.6 (s, C-8), δ_C 39.3 (s, C-10)], and

carbonyl group at δ_C 198.1 (s, C-13). The chemical structure of **2** was also confirmed by COSY and HMBC spectroscopies. In the COSY spectra, the presence of a skeletal bisnorlabdane was determined, due to cross peaks of three consecutive methylene protons H-1/H-2/H-3, two methylene protons H-6/H-7, two olefinic protons H-11/H-12. In the HMBC spectra, selective key correlations between of H-18 and H-19/C-4, H-20/C-10, and H-14/C-13, have assigned the positions of methyl groups (Figure 1). In addition, the connectivity of exomethylene group and ring at C-8, which was observed by correlations of H-17/C-7, C-8 and C-9. In the same manner, the linkage between the α, β-unsaturated ketone side chain and the ring at C-9 was improved by correlations of H-11/C-8, C-9, and C-10. By comparison of the spectroscopic data with those in published literature, compound **2** was identified as amoxantin A [9].

Compound **3** was isolated as colourless crystals. The ^{1}H-NMR of **3** showed the presence of a sesquiterpene of carotane skeleton, including, one methyl group at δ_H 1,15 (s, 7-CH_3), and two methyl protons of isopropyl group at [δ_H 0.94 (d, J = 7.0 Hz, H-13), δ_H 1.02 (d, J = 6.5 Hz, H-12)], three methylene protons at [δ_H 1.68 (m, H_a-8), δ_H 1.71 (m, H_a-9), δ_H 1.78 (m, H_b-8), δ_H 1.92 (d, J = 12.0 Hz, H_a-6), δ_H 2.02 (d, J = 12.0 Hz, H_b-6), δ_H 2.06 (m, H_b-9)], three methine protons at [δ_H 2.14 (dd, J = 7.5, 3.0 Hz, H-10), δ_H 2.41 (m, H-11), δ_H 4.02 (d, J = 5.0 Hz, H-2)], and olefinic proton at δ_H 6.63 (d, J = 5.0 Hz, H-3). The ^{13}C-NMR/DEPT data indicated a total number of 15 carbons, comprising characteristic signals of a sesquiterpene, due to three methyl carbons at [δ_C 20.7 (q, C-13), δ_C 24.8 (q, 7-CH_3), δ_C 25.8 (q, C-12)], three methylene carbons at [δ_C 24.4 (t, C-9), δ_C 45.3 (t, C-8), δ_C 57.1 (t, C-6)], four methine carbons at [δ_C 26.1 (d, C-11), δ_C 54.0 (d, C-10), δ_C 66.4 (d, C-2), δ_C 134.2 (d, C-3)], and five quaternary carbons at [δ_C 49.7 (s, C-7), δ_C 97.8 (s, C-1), δ_C 103.2 (s, C-5), δ_C 141.4 (s, C-4), δ_C 173.5 (s, CO)]. The observed correlations of methyl proton 7-CH_3/C-1, C-6, C-7, and C-8 in the HMBC spectra have determined the position of 7-CH_3 group at C-7, whereas the lingkage position of isopropyl group at C-10 was determined by correlations between H-12 and H-13/C-10 and C-11. Furthermore, the linkage of carboxyl group and olefinic carbon C-4 was determined from the correlations of H-3/C-1, C-2, and C-5. From 1D, 2D-NMR and literature data, compound **3** was identified to be rugosic acid B [10].

Compound **4** (the mixture of **4a** and **4b**) was isolated as a yellowish oil. Based on the ^{1}H-NMR and ^{13}C-NMR/DEPT spectral data, compound **4** was identified as a *vicinal*-diols. In the ^{1}H-NMR spectrum, superimpose doublet signal at δ_H 1.16 (J = 6.0 Hz) was due to two methyl groups H-1 and H-4, whereas superimpose multiple signal at δ_H 3.56 was of two hydroxygenated-methine protons H-2 and H-3. Furthermore, the ^{13}C-NMR spectrum clearly showed the appearances of four carbon signals at [δ_C 18.6 (q, C-1), δ_C 18.7 (q, C-4), δ_C 72.6 (d, C-2), and δ_C 72.7 (d, C-3)]. By comparison of the NMR data with those reported in the publication, compound **4** was determined as a mixture of enatiomers [(*2R, 3R*)-2,3-butanediol (**4a**) and (*2S, 3S*)-2,3-butanediol (**4b**)] [11].

Compound **5** was isolated as a yellowish oil. The ^{1}H-NMR data of **5** was similar to those of **4**, showing the existence of a symmetric polyalcohol. Two symmetric methyl groups H-1 and H-4 was founded at δ_H 1.14 (J = 6.5 Hz, d), while two hydroxygenated-methine protons H-2 and H-3 were characterized with multiple signals, at δ_H 3.53. Unlike compounds **4a** and **4b**, only two signals with strong intensity were observed in the ^{13}C-NMR/DEPT spectra of **5**, at δ_C 18.7 (q, C-1, C-4), and δ_C 72.7 (d, C-2, C-3)]. Those data suggest compound 5 having an internal plane of symmetry. Therefore, from above mention and literature research, the chemical structure of **5** was confirmed as *meso*-2,3-butanediol [12].

Compound **6** was obtained as white needle crystals. The ^{1}H-NMR spectrum data clearly indicated that this compound displayed as a pattern of 3,4-disubstituted benzoic acid, including ABX aromatic protons at [δ_H 6.86 (d, J = 8.5 Hz, H-5), δ_H 7.58 (d, J = 2.5, 8.5 Hz, H-6) and δ_H

7.57 (d, J = 2.5 Hz, H-2)], one methoxy group at δ_H 3.91 (4-OCH_3, s). In accordance with ^{1}H-NMR spectrum data, ^{13}C-NMR/DEPT spectrum data of **6** exhibited eight carbons, comprising one methoxy carbon at δ_C 56.4 (4-OCH_3), three aromatic carbons at [δ_C 113.8 (d, C-5), δ_C 125.3 (d, C-6) and δ_C 115.8 (d, C-2)], three quaternary carbons at [δ_C 123.1 (s, C-1), δ_C 148.7 (s, C-3) and δ_C 152.7 (s, C-4)], and a carbonyl group in the downfield, at δ_C 170.0 ppm. From above mentions and a comparison with literature data, compound **6** was determined as a derivative of benzoic acid, named 3-hydroxy-4-methoxybenzoic acid [13].

4. CONCLUSION

From the rhizomes of *Curcuma singularis* Gagnep. (Zingiberaceae), six compounds, including 3 terpenoids, *p*-menthane-1,2,4-triol (**1**), amoxantin A (**2**), rugosic acid B (**3**), 2 diols, 2,3-butanediol (**4**) [*2R,3R*-butanediol (**4a**) and *2S,3S*-butanediol (**4b**)], *meso*-2,3-butanediol (**5**), along with 3-hydroxy-4-methoxybenzoic acid (**6**) were obtained. All of six compounds were isolated for the first time from the *Curcuma* genus. The structures of those compounds were determined by 1D and 2D-NMR spectroscopic data.

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TÓM TẮT

BƯỚC ĐẦU NGHIÊN CỨU THÀNH PHẦN HÓA HỌC THÂN RỄ CÂY *CURCUMA SINGULARIS*

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Từ thân rễ loài *Curcuma singularis* Gagnep. (Zingiberaceae), sáu hợp chất bao gồm ba hợp chất terpenoit, *p*-menthane-1,2,4-triol (**1**), amoxantin A (**2**), axit rugosic B (**3**), hỗn hợp hai diol, 2,3-butanediol (**4**) [*2R,3R*-butanediol (**4a**) và *2S,3S*-butanediol (**4b**)], *meso*-2,3-butanediol (**5**) và một dẫn xuất của axit benzoic 3-hydroxy-4-methoxybenzoic acid (**6**) đã được phân lập. Sáu hợp chất trên được phát hiện lần đầu tiên từ chi *Curcuma*. Cấu trúc hóa học của các hợp chất **1-6** được xác định dựa trên các dữ kiện phổ 1D và 2D-NMR.

Từ khóa: *Curcuma singularis* Gagnep., Zingiberaceae, thân rễ, tecpenoit, labdadien, butanediol, axit benzoic.